Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Material for 'An Assessment of Vapour Pressure Estimation Methods'

90 compounds comprised the test set, they are listed in table 1, along with their CAS code, literature source, vapour pressure, temperature range and the source for their parent hydrocarbon vapour pressure, if this were found in the literature. Also listed are the sources for enthalpies of fusion, heat capacities for the solid and liquid state, and melting temperature, when these were found in the literature.

Compound	CAS code	P^0_{lors}Source	P^0_l (Pa) range	T range (K)	P^0_{hc} (Pa)✤	ΔH_{fus}	ΔC_p	T_m
Tridecanoic acid	638-53-9	*a*	2.87E-3	298.15	*b*	*c*	*c*	*d*
Tetradecanoic acid	544-63-8	*a*	1.46E-3	298.15	*e*	*c*	*c*	*d*
Pentadecanoic acid	1002-84-2	*a*	6.98E-4	298.15	*b*	*c*	*c*	*d*
Hexadecanoic acid	57-10-3	*a*	2.97E-4	298.15	*e*	*f*	*f*	*d*
Heptadecanoic acid	506-12-7	*a*	1.88E-4	298.15	*b*	*c*	*c*	*d*
Octadecanoic acid	57-11-4	*a*	6.61E-5	298.15	*g*	*f*	*f*	*d*
Nonadecanoic acid	646-30-0	*a*	3.32E-5	298.15	*e/b*	*c*	*c*	*d*
Eicosanoic acid	506-30-9	*a*	1.34E-5	298.15	*g/h*	*c*	*c*	*i*
Oxalic acid	144-62-7	*j*	2.74E-2	298.00	*k*	*j*	*j*	*j*
Malonic acid	141-82-2	*j/l/m*	3.19E-3/3.73E-1-357.494/2.07E-3	298.00/339.299-357.494/296.00	*n*	*j*	*j*	*j*
2-methyl malonic acid	516-05-2	*j/o*	5.34E-3/1.44E-1	298.00/298.00	*p*	*j*	*j*	*j*
2-hydroxy malonic acid	80-69-3	*j*	5.64E-3	298.00	*n*	*j*	*j*	*j*
Succinic acid	110-15-6	*j/q/m*	3.86E-3/1.21-4.30/1.39E-3	298.00/360.106-375.135/296.00	*r/s*	*j*	*j*	*j*
2-methyl succinic acid	498-21-5	*j/q/o*	5.58E-4/2.40E-1-1.76/3.51E-3	298.00/343.119-360.112/298.00	*t*	*j*	*j*	*j*
2-methyl, 2-hydroxy succinic acid	6236-10-8	*j*	7.48E-3	298.00	*t*	*j*	*j*	*j*
2-hydroxy succinic acid	6915-15-7	*j*	8.72E-4	298.00	*r/s*	*j*	*j*	*j*
2,3-dihydroxy succinic acid	133-37-9	*j*	3.23E-1	298.00	*r/s*	*j*	*j*	*j*
2-amino succinic acid	56-84-8	*j*	2.56E-2	298.00	N/A	*j*	*j*	*j*
2-keto succinic acid	328-42-7	*j*	1.67E-2	298.00	*r/s*	*j*	*j*	*j*
Glutaric acid	110-94-1	*j/l/m*	1.96E-3/0.3404-1.334/3.3E-3	298.00/348.150-363.149/296.00	*u*	*v*	*v*	*j*
2-methyl glutaric acid	617-62-9	*j/q*	9.63E-4/1.28E-1-4.299E-1	298.00/338.378-347.643	*LK_P*	*j*	*j*	*j*
3-methyl glutaric acid	626-51-7	*j/o*	9.19E-4/3.8E-3	298.00/298.00	*LK_P*	*j*	*j*	*j*
3-carboxylic, 3-hydroxy glutaric acid	77-92-9	*j*	3.10E-3	298.00	*LK_P*	*j*	*j*	*j*
2-amino glutaric acid	56-86-0	*j*	2.05E-3	298.00	N/A	*j*	*j*	*j*
2-keto glutaric acid	328-50-7	*j*	2.02E-3	298.00	*u*	*j*	*j*	*j*
3-keto glutaric acid	542-05-2	*j*	3.22E-3	298.00	*u*	*j*	*j*	*j*
Adipic acid	124-04-9	*j/m/o*	2.14E-4/3.7E-4/5.7E-4	298.00/296.00/298.00	*u*	*v*	*v*	*j*
Suberic acid	505-48-6	*v/m*	2.23E-5/2.4E-5	298.00/296.00	*b*	*w*	*w*	*w*
ortho-phthalic acid	88-99-3	*x*	1.68E-3	298.00	N/A	*x*	*x*	*x*
meta-isophthalic acid	121-91-5	*x*	1.40E-2	298.00	N/A	*x*	*x*	*x*
para-terephthalic acid	100-21-0	*x*	1.38E-1	298.00	N/A	*y*	*y*	*y*
1,1-cyclopropane dicarboxylic acid	598-10-7	*v*	3.10E-3	298.00	LK_P	*v*	*v*	*v*
1,1-cyclobutane dicarboxylic acid	5445-51-2	*v*	6.47E-3	298.00	LK_P	*v*	*v*	*v*
1,2-cyclopentane dicarboxylic acid	1461-96-7	*v*	3.47E-4	298.00	LK_P	*v*	*v*	*v*

1,3-cyclohexane dicarboxylic acid	3971-31-1	*v*	4.60E-4	298.00	LK_P	*v*	*v*	*v*
Azelaic acid	123-99-9	*l*/*m*	1.287E-1-3.722E-1/8.1E-5	367.062-377.038/296.00	*b*	*z*	*z*	*l*
Undecanedioc acid	1852-04-6	*l*	7.933E-2-2.146E-1	371.184-380.925	*b*	*z*	*z*	*l*
Dodecanedioc acid	1852-04-6	*a*	2.27E-4	298.00	*b*	*z*	*z*	*z*
cis-pinonic acid	473-72-3	*v*	7.78E-4	298.00	LK_P	*v*	*v*	*v*
para-anisic acid	100-09-4	*x*	4.76E-3	298.00	N/A	*x*	*x*	*x*
Vanillic acid	121-34-6	*x*	1.42E-3	298.00	N/A	*x*	*x*	*x*
Syringic acid	530-57-4	*x*	9.80E-4	298.00	N/A	*x*	*x*	*x*
Nitrocatechol	3316-09-4	*x*	9.99E-4	298.00	N/A	*x*	*x*	*x*
Levoglucosan	498-07-7	*v*	1.35E-4	298.00	N/A	*v*	*v*	*v*
ortho-dimethyl amino benzoic acid	610-16-2	*x*	1.07E-2	298.00	N/A	*x*	*x*	*x*
meta-dimethyl amino benzoic acid	99-64-9	*x*	6.42E-4	298.00	N/A	*x*	*x*	*x*
1,2-pentanediol	5345-92-0	*a*1	1.35-98.44	289.2-336.2	*u*	N/A	N/A	N/A
1,2,3-trihydroxypropane	56-81-5	*a*2	0.0249-1.97	298.75-341.35	*n*	N/A	N/A	N/A
1,4-butanediol	110-63-4	*a*3	13.85-84.55	329.2-351.2	*r*/*s*	N/A	N/A	
2-(methylamino)ethanol	109-83-1	*a*4	13.94 - 92.12	274.9-296.3	N/A	N/A	N/A	N/A
2,4-pentanediol	625-69-4	*a*5	4.8-87.35	297.2-330.5	*u*	N/A	N/A	N/A
2,6-dinitrotoluene	606-20-2	*a*6	0.0127-1.974	277.15-323.15	N/A	*a*7	*a*7	*a*7
2-aminoethanol	141-43-5	*a*4	8.48-83.66	279.0-306.3	N/A	N/A	N/A	*a*4
2-aminonitrobenzene	88-74-4	*a*8	1.20-12.37	313.5-342.3	N/A	*a*9	*a*9	*a*9
2-chloro-3,5-dimethoxy-4-HBA	76341-69-0	*a*10	0.046-0.9	293.15-323.15	N/A	N/A	N/A	N/A
2-chloropropionic acid	598-78-7	*a*11	13.36-82.72	287.4-308.4	N/A	N/A	N/A	N/A
2-hydroxybenzoic acid	69-72-7	*a*12	0.443-2.434	307.05-323.71	N/A	*a*9	*a*9	*a*9
2-phenylbromide-TEGMME	929259-37-0	*a*13	0.061-1.446	333.2-369.9	N/A	N/A	N/A	N/A
3-(2-methoxyphenyl)PA	6342-77-4	*a*14	0.329-1.514	331.156-347.165	N/A	*a*14	N/A	*a*14
3-(3,4-dimethoxyphenyl)PA	2107-70-2	*a*14	0.1159-0.4707	352.178-366.163	N/A	*a*13	N/A	*a*14
3,4-dichloronitrobenzene	99-54-7	*a*15	9.1-74.69	316.3-346.5	N/A	N/A	N/A	*a*15
3,4-dihydroxychlorobenzene	99-54-7	*a*10	0.6-8.7	293.15-323.15	N/A	N/A	N/A	*a*16
3,5-di-tert-butylcatechol	1020-31-1	*a*17	0.270-5.58	313.2-346.2	N/A	*a*17	est	*a*17
3,7-dimethyl-7-hydroxyoctanol	107-75-5	*a*17, *a*18	0.117-15.87	283.355-332.65	LK_P	N/A	N/A	N/A
3-chloro-2,6-dimethoxyphenol	18113-22-9	*a*10	0.52-7.1	293.15-323.15	N/A	N/A	N/A	*a*19
3-chloroaminobenzene	108-42-9	*a*15	6.02-76.82	291.2-325.3	N/A	N/A	N/A	*a*15
3-hydroxypropanenitrile	109-78-4	*a*20	15.64-91.47	306.3-331.4	N/A	N/A	N/A	*a*21
3-nitro-3-(4-nitrophenyl)-pentane	204189-06-0	*a*8	0.063-1.920	321.4-358.1	N/A	N/A	N/A	N/A
3-nitrobenzoic acid	121-92-6	*a*22	0.604-2.03	347.16-361.16	N/A	*a*9, *a*23	*a*24, est	*a*9
3-nitrophenol	554-84-7	*a*25	14.74-35.51	357.2-369.3	N/A	*a*25	N/A	*a*25
4-aminobenzoic acid	150-13-0	*a*26	0.28-2.31	359.14-382.56	N/A	*a*9	est.	*a*9, *a*27
Anisaldehyde	123-11-5	*a*17, *a*18	1.32-30.4	283.95-322.95	N/A	N/A	N/A	*a*28
Benzyl salicylate	118-58-1	*a*17, *a*18	0.016-1.24	295.45-342.95	N/A	N/A	N/A	*a*17
Dibutyl phthalate	84-74-2	*a*29	0.00191-0.0335	293.05-317.15	N/A	N/A	N/A	*a*30
Ethyl vanillin	121-32-4	*a*18, *a*31	0.96-3.78	323.35-337.45	N/A	*a*32	N/A	*a*32
Eugenol	97-53-0	*a*18, *a*33	0.64-20.00	285.45-326.75	N/A	N/A	N/A	*a*21

Glycerine carbonate	931-40-8	$a34$	0.29-46.94	330.2-398.5	N/A	N/A	N/A	N/A
Heliotropin	120-57-0	$a18$, $a31$	0.58-11.60	293.45-326.85	N/A	est	N/A	$a18$
Isoamyl salicylate	87-20-7	$a17$, $a18$	0.22-8.93	287.95-328.55	N/A	N/A	N/A	N/A
1'-hydroxy-1,1'-bi(cyclohexyl)-2-one	28746-99-8	$a35$	1.23-6.64	308.22-330.4	LK_P	N/A	N/A	$a35$
Methyl anthranilate	134-20-3	$a18$, $a36$	2.32-13.73	299.45-319.15	N/A	N/A	N/A	$a18$, $a36$
Musk Ambrette	83-66-9	$a18$, $a31$	0.303-1.33	328.55-345.45	N/A	est	N/A	$a18$, $a31$
N-methyldiethanolamine	105-59-9	$a37$	0.61-80.9	293.69-353.0	N/A	N/A	N/A	N/A
1-(4-Methoxyphenyl)ethanone	100-06-1	$a36$	5.60-25.5	313.55-333.45	N/A	N/A	N/A	$a36$
1,3,5-benzenetriol	108-73-6	$a38$	0.82-5.06	381.31-404.58	N/A	$a1$	est	$a1$
Pimelic acid	111-16-0	$v/l/m$	2.6E-4/1.928E-1-7.761E-1/3.4E-4	298.00/358.149-371.656/296.00	b	w, $a39$	w, $a39$	l, $a39$
Pinonaldehyde	2704-78-1	$a40$	0.09-0.6	263.15-278.15	LK_P	N/A	N/A	N/A
Tetraethylene glycol	112-60-7	$a41$	0.173-44.7	323.23-398.23	N/A	N/A	N/A	$a21$
Triacetin	102-76-1	$a42$	0.0512-2.081	284.2-318.2	N/A	N/A	N/A	$a21$
Triethylene glycol dinitrate	111-22-8	$a42$	0.025-2.21	303.4-348.0	N/A	N/A	N/A	N/A

Table 1: a = Chattopadhyay and Ziemann (2005), b = Ambrose and Walton (1989), c = Schaake et al. (1982a), d=Gaikwad and Subrahmanymam (1985), e = Morgan and Kobayashi (1994), f = Schaake et al. (1982b), g = Macknick and Prausnitz (1979), h = Chirico et al. (1989), i = Adriaanse et al. (1964), j = Booth et al. (2010), k=Straty and Tsumura (1976), l=da Silva et al. (1999b), m= Bilde et al. (2003), n = Kratzke (1980), o = Mønster et al. (2004), p = Aston et al. (1940), q = da Silva et al. (2001), r = Flebbe et al. (1982), s = Martínez-Ortiz and Manley (1978), t = Schumann et al. (1942), u = Ewing and Ochoa (2006), v = Booth et al. (2011), LK_P = Reid et al. (1987), w = Roux et al. (2005), x = Booth et al. (2012), y = Huang et al. (2009), z = Cingolani and Berchiesi (1974), $a1$ = Verevkin (2004), $a2$ = Cammenga et al. (1977), $a3$ = Vasiltsova et al. (2005), $a4$ = Kapteina et al. (2005), $a5$ = Verevkin (2007), $a6$ = Pella (1977), $a7$ = Finch and Payne (1990), $a8$ = Verevkin (1997), $a9$ = Domalski and Hearing (2006), $a10$ = Lei et al. (1999), $a11$ = Lagoa et al. (2002), $a12$ = Colomina (1981), $a13$ = Dabrowska et al. (2006), $a14$ = Monte and Hillesheim (2001), $a15$ = Verevkin and Schick (2003), $a16$ = Parke and Williams (1955), $a17$ = Serpinskii et al. (1955), $a18$ = Serpinskii et al. (1958), $a19$ = Varhanickova et al. (1958), $a20$ = Roux et al. (2007), $a21$ = Dykyi and Repas (1979), $a22$ = da Silva et al. (1999a), $a23$ = Rai and Mandal (1990), $a24$ = Andrews (1926), $a25$ = Heintz et al. (2007), $a26$ = Dekruif et al. (1979), $a27$ = Andrews et al. (1926), $a28$ = Kendall and Gibbons (1915), $a29$ = Birks and Bradley (1949), $a30$ = Song et al. (2003), $a31$ = Serpinskii et al. (1953), $a32$ = Skerget et al. (2005), $a33$ = Serpinskii et al. (1957), $a34$ = Verevkin et al. (2008), $a35$ = Shevelyova et al. (2006), $a36$ = Serpinskii et al. (1954), $a37$ = Noll (1998), $a38$ = de Wit et al. (1983), $a39$ = Steele et al. (2002), $a40$ = Hallquist et al. (1997), $a41$ = Hales et al. (1981), $a42$ = Woodman and Adicoff (1963). ✣ N/A denotes chemicals that have a group not specified in the Capouet and Muller (2006) method and thus do not require P^0_{hc}.

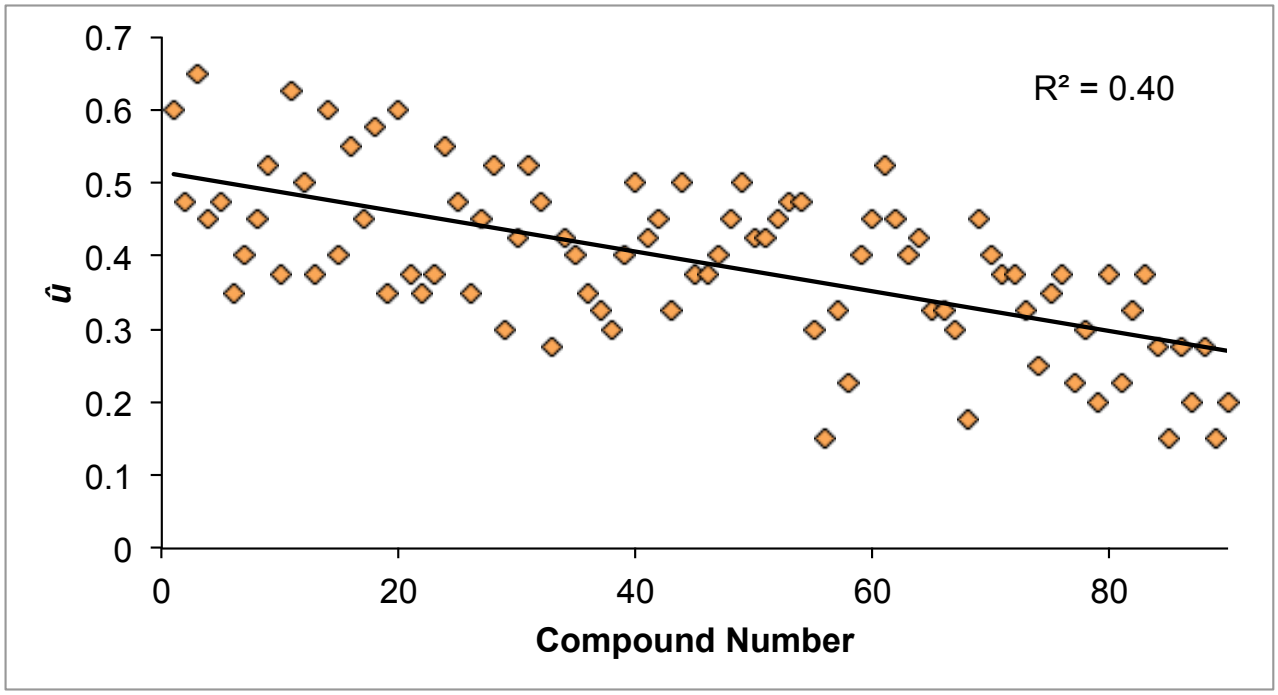

Figure 1: The metric accounting for hydrogen bond number and carbon number (eq. 17 of the main report) ordered by the maximum absolute error of a given compound (i.e., same order as Fig. 5 in the main report).

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